Solving PDEs on Overlapping Grids with Overture

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Current Overture developers

Kyle Chand

Bill Henshaw

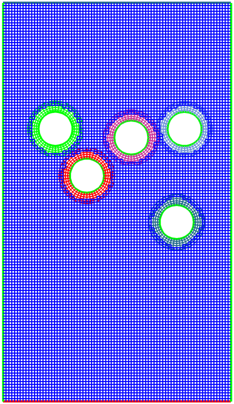
Major Contributors

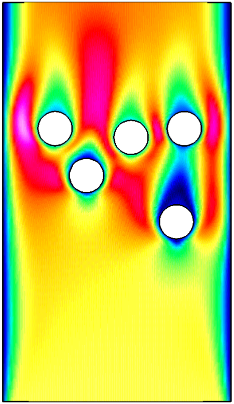
Don Schwendeman (RPI),

Jeff Banks (LLNL).

What are overlapping grids and why are they useful?

Overlapping grid: a set of structured grids that overlap.





- Overlapping grids can be rapidly generated as bodies move.
- High quality grids under large displacements.
- Cartesian grids for efficiency.
- Efficient for high-order accurate methods.

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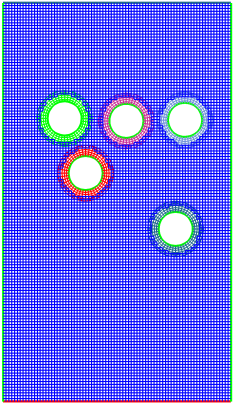

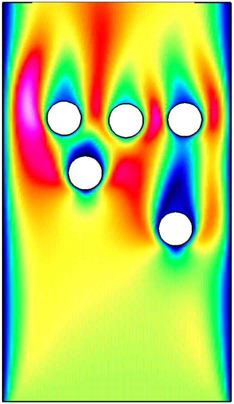

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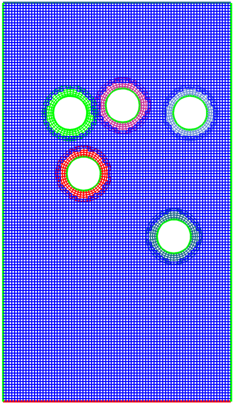

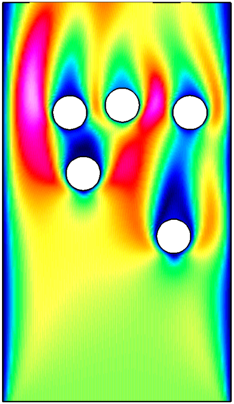

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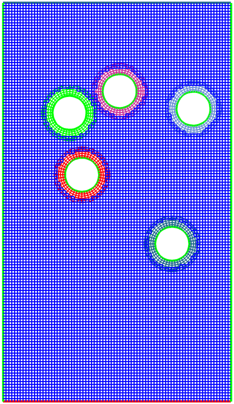

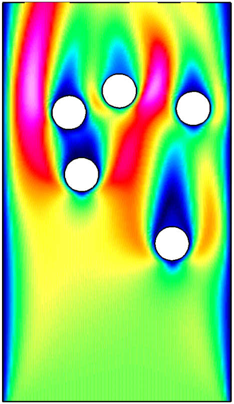

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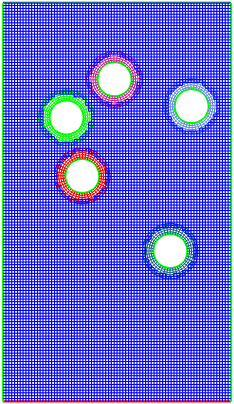

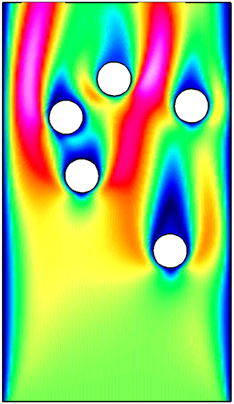

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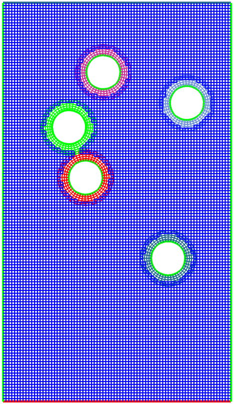

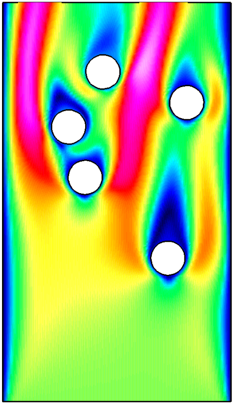

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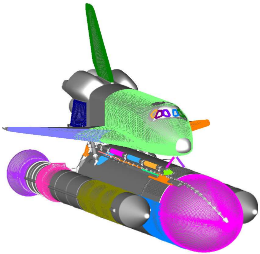
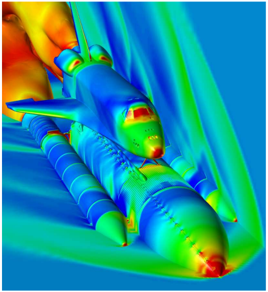
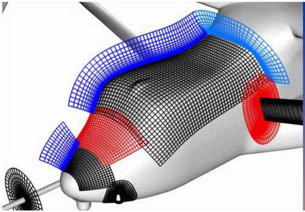
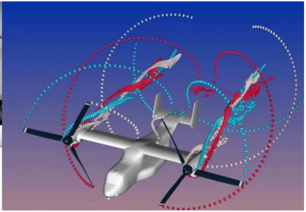
Aerospace applications using overlapping grids.









Space shuttle figures courtesy of William Chan and Reynaldo Gomez.
V-22 Osprey figures courtesy of William Chan, Andrew Wissink and Robert Meakin.

Overture: tools for solving PDE's on overlapping grids

- high level C++ interface for rapid prototyping of PDE solvers.
- built upon optimized C and fortran kernels.
- library of finite-difference operators: conservative and non-conservative, 2nd, 4th, 6th and 8th order accurate approximations.
- support for moving grids.
- support for block structured adaptive mesh refinement (AMR).
- extensive grid generation capabilities (Ogen).
- CAD fixup tools (for CAD from IGES files).
- interactive graphics and data base support (HDF).

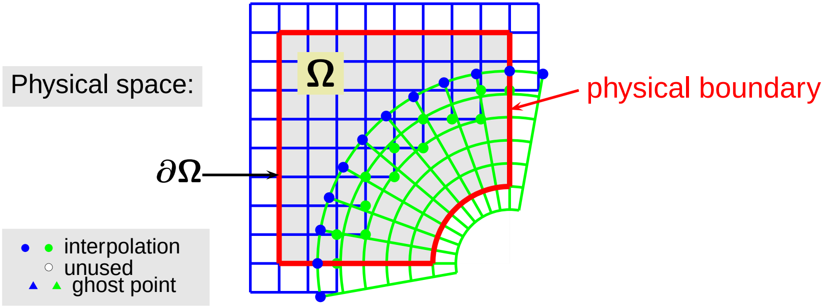
The CG (Composite Grid) suite of PDE solvers

- cgad: advection diffusion equations.
- cgins: incompressible Navier-Stokes with heat transfer.
- cgcns: compressible Navier-Stokes, reactive Euler equations.
- cgmp: multi-physics solver (e.g. conjugate heat transfer).
- cgmx: time domain Maxwell's equations solver.
- cgsm: solid mechanics (*new*)

Overture and CG are freely available from the web:

www.llnl.gov/CASC/Overture

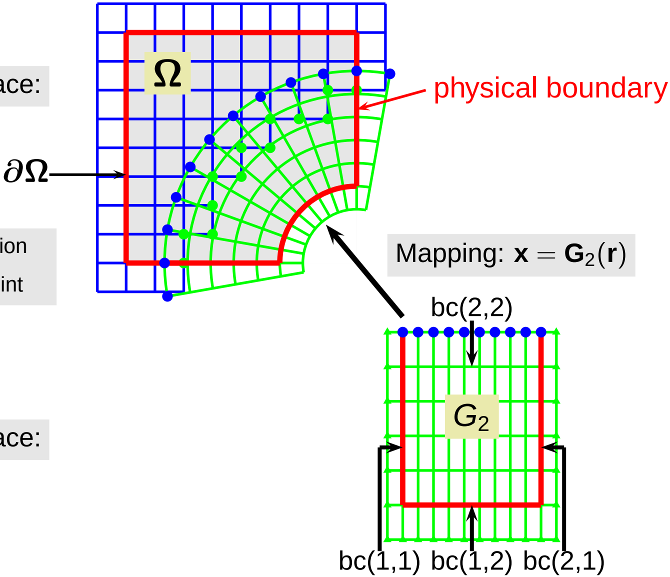
Components of an Overlapping Grid



Components of an Overlapping Grid

Physical space:

- interpolation
- unused
- ghost point



Parameter space:

Component grid 2

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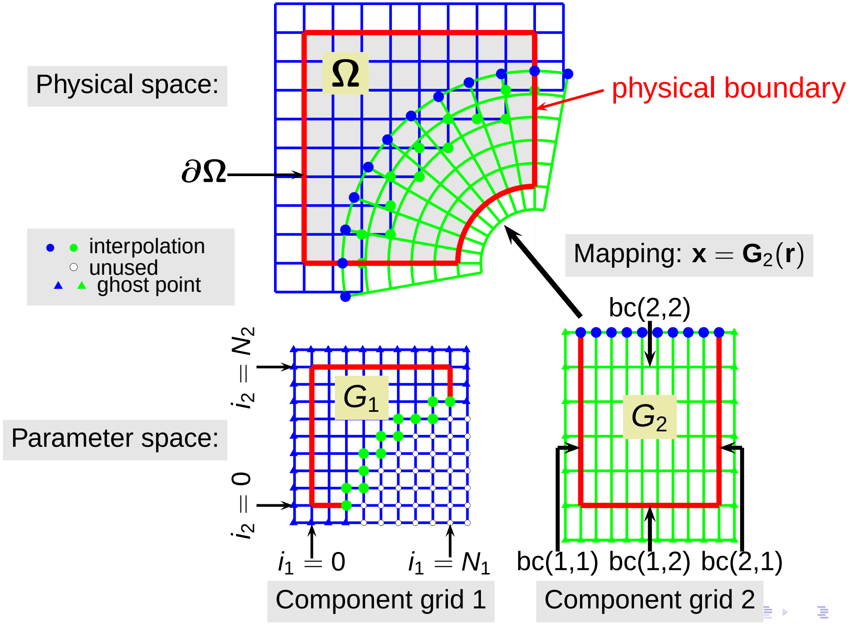
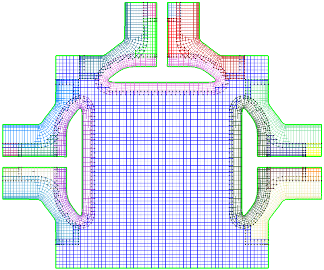
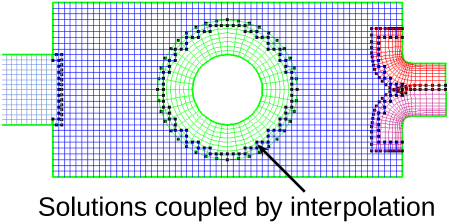
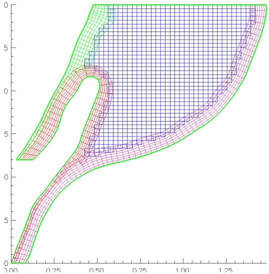


Ogen can be used to build 2D overlapping grids:







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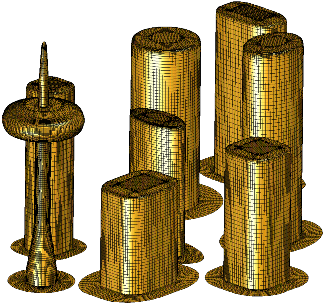

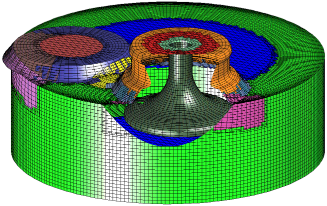

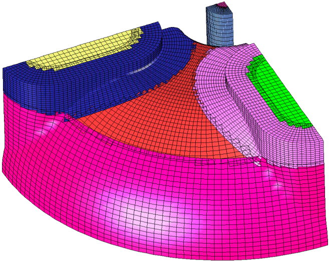

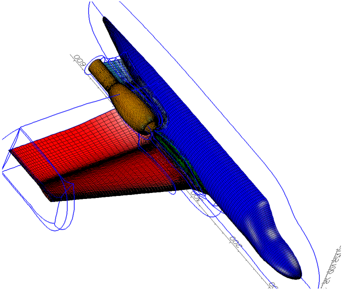

Composite/ Chimera/ Overset/ Overlapping Grids

A Short History

- Volkov, circa [1966] developed a *Composite Mesh* method for Laplace's equation on regions with piece-wise smooth boundaries separated by corners. Polar grids are fitted at corners to handle potential singularities.
- Starius, circa [1977] (student of H.-O. Kreiss) considered *Composite Mesh* methods for elliptic and hyperbolic problems – introduces a hyperbolic grid generator.
- Steger, circa [1980] independently conceives the idea of the overlapping grid, subsequently named the *Chimera* approach after the mythical Chimera beast having a human face, a lion's mane and legs, a goat's body, and dragon's tail. NASA groups develop grid generator PEGSUS, hyperbolic grid generation and flow solver Overflow (Steger, Benek, Suhs, Buning, Chan, Meakin, et. al.)
- B. Kreiss circa [1980] develops overlapping grid generator which subsequently leads to the CMPGRD grid generator [1983] (Chesshire, Henshaw) later leading to the Overture set of tools [1994].

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Theory for finite difference schemes

There is extensive numerical analysis theory underpinning this work.

- classic von Neumann stability analysis (periodic domains).
- energy estimates (L_2-norm estimates).
- normal mode analysis, GKS theory (initial boundary value problems).

Some references:

- Gustafsson, Kreiss, Oliger, *Time Dependent Problems and Difference Methods*, (book).
- Strikwerda, *Finite Difference Schemes and Partial Differential Equations*, (book).
- Gustafsson, Kreiss, Sundström, *Stability Theory of Difference Approx. for Mixed Initial Boundary Value Problems, I. and II.*, Math. Comp.
- Starius, *On Composite Mesh Difference Methods for Hyperbolic Differential Equations*, Numer. Math.

A one-dimensional overlapping grid example

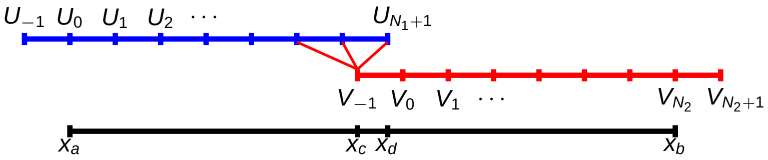
To solve the advection-diffusion equation

$$\begin{aligned} u_t + a u_x &= \nu u_{xx}, && x \in (0,1) \\ u(0,t) = g_0(t), \quad u_x(1,t) &= g_1(t), && \text{(boundary conditions)} \\ u(x,0) &= u_0(x), && \text{(initial conditions)} \end{aligned}$$

introduce grid points on the two overlapping component grids,

$$\begin{aligned} x_i^{(1)} &= x_a + i\Delta x_1, & i &= -1,0,1,\ldots,N_1+1, & \Delta x_1 &= (x_d - x_a)/N_1 \\ x_j^{(2)} &= x_c + (j+1)\Delta x_2, & j &= -1,0,1,\ldots,N_2+1, & \Delta x_2 &= (x_b - x_c)/N_2 \end{aligned}$$

and approximations $U_i^n \approx u(x_i^{(1)}, n\Delta t)$, $V_i^n \approx u(x_i^{(2)}, n\Delta t)$.



Discretize with forward-Euler and central differences

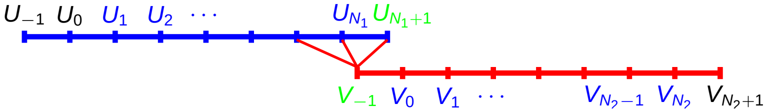
Given the solution at time t^n, compute the solution at time t^{n+1}:

$$
\begin{aligned}
(U_i^{n+1} - U_i^n)/\Delta t &= -aD_0 U_i^n + \nu D_+ D_- U_i^n, \qquad i = 1, 2, \ldots, N_1 \\
(V_j^{n+1} - V_j^n)/\Delta t &= -aD_0 V_j^n + \nu D_+ D_- V_j^n, \qquad j = 0, 2, \ldots, N_2 \\
U_0^{n+1} &= g(t^n), \quad D_0 V_{N_2}^{n+1} = g_1(t^{n+1}), \qquad \text{(boundary conditions)}
\end{aligned}
$$

$$
U_{N_1+1}^{n+1} = (1-\alpha)(1-\frac{\alpha}{2})\, V_{-1}^{n+1} + \alpha(2-\alpha)\, V_0^{n+1} + \frac{\alpha}{2}(\alpha - 1)\, V_1^{n+1}, \quad \text{(interpolation)}
$$

$$
V_{-1}^{n+1} = (1-\beta)(1-\frac{\beta}{2})\, U_{N_1-1}^{n+1} + \beta(2-\beta)\, U_{N_1}^{n+1} + \frac{\beta}{2}(\beta - 1)\, U_{N_1+1}^{n+1}, \quad \text{(interpolation)}
$$

$$
D_0 U_i^n = \frac{U_{i+1}^n - U_{i-1}^n}{2\Delta x}, \quad D_+ U_i^n = \frac{U_{i+1}^n - U_i^n}{\Delta x}, \quad D_- U_i^n = \frac{U_i^n - U_{i-1}^n}{\Delta x}.
$$



Overture supports a high-level C++ interface

But is built upon mainly Fortran kernels.

Solve $u_t + au_x + bu_y = \nu(u_{xx} + u_{yy})$

```
CompositeGrid cg;     // create a composite grid
getFromADataBaseFile(cg,"myGrid.hdf");
floatCompositeGridFunction u(cg);     // create a grid function
u=1.;
CompositeGridOperators op(cg);    // operators
u.setOperators(op);
float t=0, dt=.005, a=1., b=1., nu=.1;
for( int step=0; step<100; step++ )
{
   u+=dt*( -a*u.x()-b*u.y()+nu*(u.xx()+u.yy()) );     // forward Euler
   t+=dt;
   u.interpolate();
   u.applyBoundaryCondition(0,dirichlet,allBoundaries,0.);
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}
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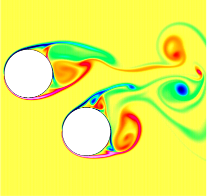
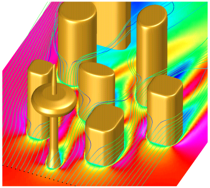
Overture is used by research groups worldwide

- Blood flow in veins with blood clot filters. (Mike Singer, LLNL).
- Pitching airfoils and micro-air vehicles (Yongsheng Lian, U. of Louisville)
- Relativistic hydrodynamics and Einstein field equations (Philip Blakely, Nikos Nikiforakis, U. Cambridge).
- Compressible flow/ice-formation (Graeme Leese, U. Cambridge).
- Tear films and droplets (Rich Braun U. Delaware, Kara Maki UMN).
- High-order accurate subsonic/transonic aero-acoustics (Phillipe Lafon, CNRS, EDF, France).
- Low Reynolds flow for pitching airfoils (D. Chandar, R. Yapalparvi, M. Damodaran, NTU, Singapore).
- Incompressible flow in pumps (J.P. Potanza, Shell Oil, Houston).
- High-order accurate, compact Hermite-Taylor schemes (Tom Hagstrom, SMU, Dallas).

Cgins: incompressible Navier-Stokes solver.





- 2nd-order and 4th-order accurate (DNS).
- support for moving rigid-bodies (not parallel yet).
- heat transfer (Boussinesq approximation).
- semi-implicit (time accurate), pseudo steady-state (efficient line solver), full implicit.

• WDH., *A Fourth-Order Accurate Method for the Incompressible Navier-Stokes Equations on Overlapping Grids*, J. Comput. Phys, **113**, no. 1, (1994) 13–25.

Incompressible Navier-Stokes.

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \nu\Delta\mathbf{u} - \mathbf{f} = 0, \qquad t>0, \quad \mathbf{x}\in\Omega$$
$$\nabla\cdot\mathbf{u} = 0 \qquad t>0, \quad \mathbf{x}\in\Omega$$

Divergence damping term: $\alpha\nabla\cdot\mathbf{u}$ is important.

Wall boundary conditions:

$$\mathbf{u} = 0, \quad \nabla\cdot\mathbf{u}=0, \text{ (pressure BC)} \quad \mathbf{x}\in\partial\Omega,$$

with *numerical boundary condition*:

$$p_n = -\mathbf{n}\cdot(\,\nu\nabla\times\nabla\times\mathbf{u}\,).$$

Use $\nabla\times\nabla\times\mathbf{u}$ instead of $\Delta\mathbf{u}$ for implicit time-stepping.

- WDH, N.A. Petersson, *A Split-Step Scheme for the Incompressible Navier-Stokes Equations*, 2003.

Incompressible Navier-Stokes.

Split-step, velocity-pressure formulation:

$$\begin{aligned} \mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \nu\Delta\mathbf{u} - \mathbf{f} &= 0, \qquad t>0, \quad \mathbf{x}\in\Omega \\ \Delta p - \nabla\mathbf{u} : \nabla\mathbf{u} - \alpha\nabla\cdot\mathbf{u} - \nabla\cdot\mathbf{f} &= 0, \qquad t>0, \quad \mathbf{x}\in\Omega \end{aligned}$$

Divergence damping term: $\alpha\nabla\cdot\mathbf{u}$ is important.

Wall boundary conditions:

$$\mathbf{u} = 0, \quad \nabla\cdot\mathbf{u} = 0, \ \text{(pressure BC)} \quad \mathbf{x}\in\partial\Omega,$$

with *numerical boundary condition*:

$$p_n = -\mathbf{n}\cdot(\,\nu\nabla\times\nabla\times\mathbf{u}\,).$$

Use $\nabla\times\nabla\times\mathbf{u}$ instead of $\Delta\mathbf{u}$ for implicit time-stepping.

- WDH, N.A. Petersson, *A Split-Step Scheme for the Incompressible Navier-Stokes Equations*, 2003.

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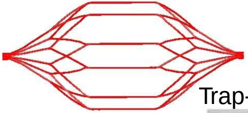
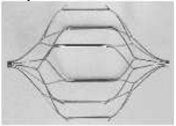
- WDH, N.A. Petersson, *A Split-Step Scheme for the Incompressible Navier-Stokes Equations*, 2003.

Flow past a blood-clot filter using cgins

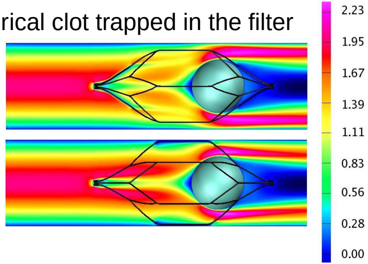
Overlapping grid for the filter



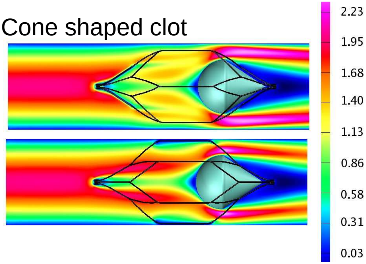
Trap-ease wire filter



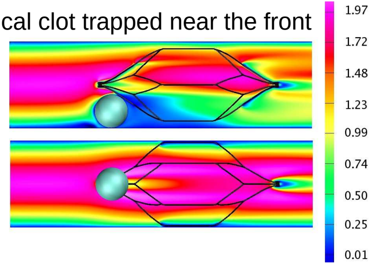
Spherical clot trapped in the filter



Cone shaped clot

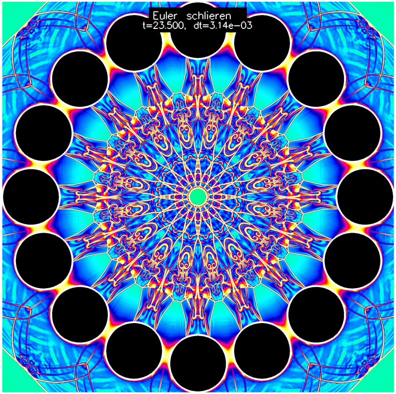


Spherical clot trapped near the front



M.A. Singer, WDH, S.L. Wang, *Computational Modeling of Blood Flow in the Trapease Inferior Vena Cava Filter*, Journal of Vascular and Interventional Radiology, **20**, 2009.

Cgcns: compressible N-S and reactive-Euler.

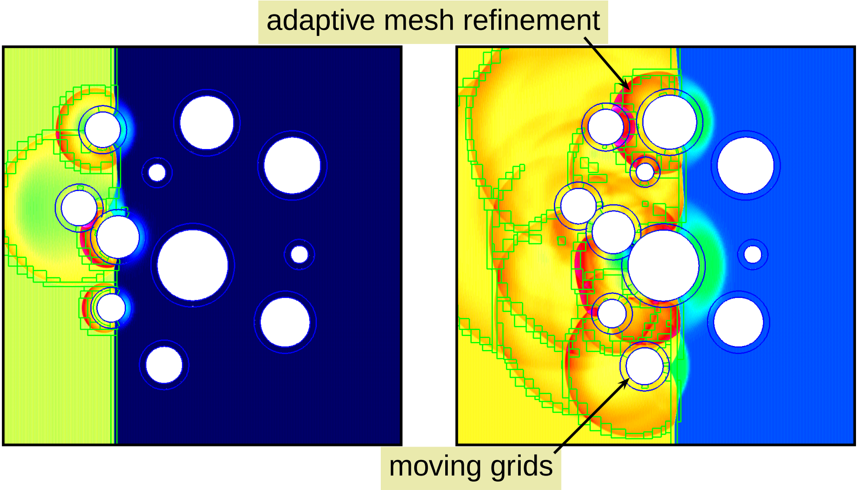


- reactive and non-reactive Euler equations, Don Schwendeman (RPI).
- compressible Navier-Stokes.
- multi-fluid formulation, Jeff Banks (LLNL).
- adaptive mesh refinement and moving grids.

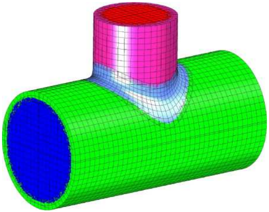
• WDH., D. W. Schwendeman, *Parallel Computation of Three-Dimensional Flows using Overlapping Grids with Adaptive Mesh Refinement*, J. Comp. Phys. **227** (2008).
• WDH., DWS, *Moving Overlapping Grids with Adaptive Mesh Refinement for High-Speed Reactive and Nonreactive Flow*, J. Comp. Phys. **216** (2005).
• WDH., DWS, An adaptive numerical scheme for high-speed reactive flow on overlapping grids, J. Comp. Phys. **191** (2003).

Moving overlapping grids and AMR

A shock hitting a collection of cylinders (density).

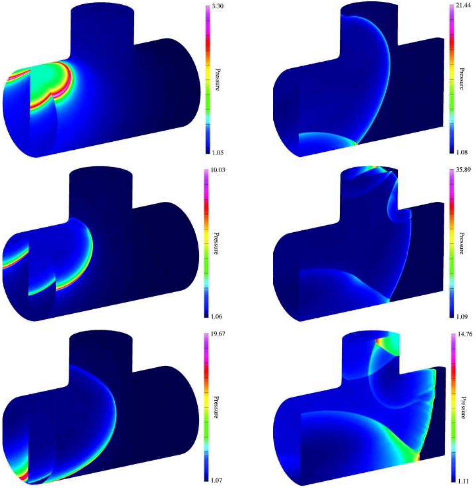


Detonation initiation in a T-shaped pipe



overlapping grid

pressure



Notes: cgcns, reactive-Euler: one refinement level, factor 4, 4930 time steps, 48 processors, from 5 to 682 grids, 100M pts (max) (eff. resolution 400 M).

Estimating Convergence Rates

Define the volume-weighted discrete L_p-norm of a grid function $U_{\mathbf{i}}$ as

$$\|U_{\mathbf{i}}\|_p = \left(\frac{\sum_{\mathbf{i}} |U_{\mathbf{i}}|^p \, d\mathcal{V}_{\mathbf{i}}}{\sum_{\mathbf{i}} d\mathcal{V}_{\mathbf{i}}}\right)^{1/p}, \qquad d\mathcal{V}_{\mathbf{i}} = \left|\frac{\partial \mathbf{x}}{\partial \mathbf{r}}\right|_{\mathbf{i}} dr_1 dr_2 dr_3.$$

Assume the discrete solution $U_{\mathbf{i}}^m$ at grid spacing h_m satisfies

$$U_{\mathbf{i}}^m - u(\mathbf{x}_{\mathbf{i}}^m, t) \approx C_{\mathbf{i}}^m h_m^\mu,$$

The difference between resolution h_n and h_m is

$$\|U_{\mathbf{i}}^m - \mathcal{R}_n^m U_{\mathbf{i}}^n\|_p \approx C|h_m^\mu - h_n^\mu|,$$

where $\mathcal{R}_n^m$ is a fine to coarse restriction operator.

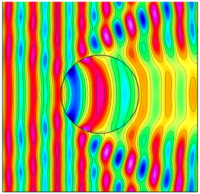
Result: Given three solutions we can estimate the convergence rate μ and the error.

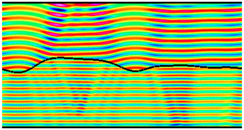
Estimating Convergence Rates

Detonation in a T-Pipe				
	$t = 2.0$		$t = 2.8$	
h_m	$\mathcal{E}_1^m$	$\mathcal{E}_2^m$	$\mathcal{E}_1^m$	$\mathcal{E}_2^m$
$1/120$	4.0e$-$3	3.0e$-$2	3.8e$-$2	2.6e$-$1
$1/160$	2.2e$-$3	1.6e$-$2	2.4e$-$2	1.9e$-$1
$1/240$	9.8e$-$4	7.1e$-$3	1.2e$-$2	1.2e$-$1
rate, μ	2.04	2.07	1.65	1.09

Estimated L_1 and L_2 errors in the density, $\mathcal{E}_1^m$ and $\mathcal{E}_2^m$, respectively, and convergence rates μ at $t = 2.0$ and $t = 2.8$.

Cgmx: electromagnetics solver.





- a time-domain finite difference scheme.
- fourth-order accurate, 2D, 3D.
- Efficient time-stepping with the modified-equation approach
- High-order accurate symmetric difference approximations.
- High-order-accurate *centered* boundary and interface conditions.

• WDH., *A High-Order Accurate Parallel Solver for Maxwell's Equations on Overlapping Grids*, SIAM J. Scientific Computing, **28**, no. 5, (2006).

Maxwell's equations are solved in second-order form

Maxwell's equations:

$$\epsilon\mu\ \partial_t^2\mathbf{E} = \Delta\mathbf{E} + \nabla\Big(\nabla \ln\epsilon\ \cdot \mathbf{E}\Big) + \nabla\ln\mu \times \Big(\nabla\times\mathbf{E}\Big) - \mu\partial_t\mathbf{j}$$

$$\epsilon\mu\ \partial_t^2\mathbf{H} = \Delta\mathbf{H} + \nabla\Big(\nabla \ln\mu\ \cdot \mathbf{H}\Big) + \nabla\ln\epsilon \times \Big(\nabla\times\mathbf{H}\Big) + \epsilon\nabla\times(\frac{1}{\epsilon}\mathbf{j})$$

Advantages of the second-order form:

- No need for a staggered grid since the operator Δ is elliptic.
- One can solve for **E** alone.

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Modified Equation time stepping

Taylor series in time:

$$\frac{u(t+\Delta t)-2u(t)+u(t-\Delta t)}{\Delta t^2} = u_{tt} + \frac{\Delta t^2}{12} u_{tttt} + O(\Delta t^4)$$

For the wave equation

$$u_{tt} = \Delta u$$

a fourth-order scheme in space and time is

$$\frac{U_i^{n+1} - 2U_i^n + U_i^{n-1}}{\Delta t^2} = \Delta_{4h} U_i^n + \frac{\Delta t^2}{12} (\Delta^2)_{2h} U_i^n$$

This scheme is very efficient (especially on Cartesian grids) and allows a large (cfl=1) time step.

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Centered numerical boundary conditions for high-order approximations

Vector wave equation on a square

$$\mathbf{E}_{tt} = \mathbf{E}_{xx} + \mathbf{E}_{yy} \quad \mathbf{x} \in \Omega = [0,1]^2$$

PEC (perfect electrical conductor) boundary at $x = 0$:

$$E^y(0,y,t) = 0 \qquad (\text{from } \mathbf{n} \times \mathbf{E} = 0),$$
$$\partial_x E^x(0,y,t) = 0 \qquad (\text{from } \nabla \cdot \mathbf{E} = 0).$$

Taking time derivatives of the above and using the equations:

$$\partial_x^{2m} E^y(0,y,t) = 0 \quad m = 0,1,2,3,\ldots$$
$$\partial_x^{2m+1} E^x(0,y,t) = 0 \quad m = 0,1,2,3,\ldots$$

These *centered* conditions are used on the boundary instead of one-sided approximations.

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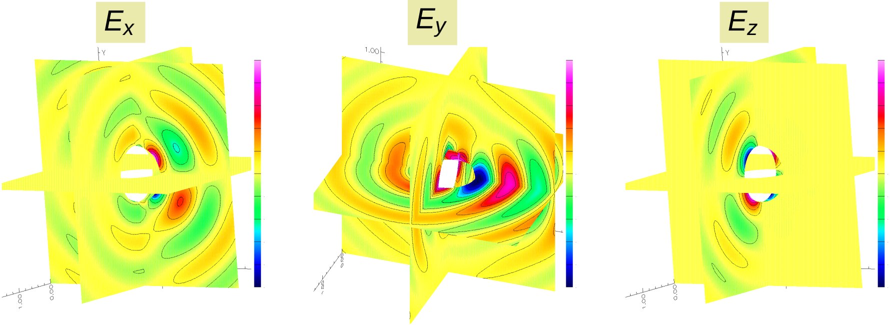
Scattering of a plane wave by a sphere

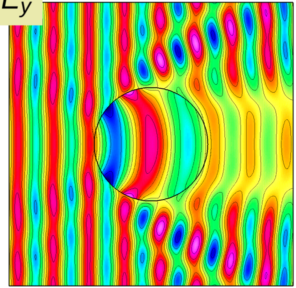


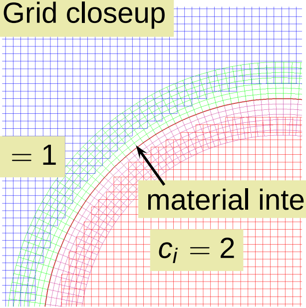
grid	N	$\|\|e^{E_x}\|\|_\infty$	$\|\|e^{E_y}\|\|_\infty$	$\|\|e^{E_z}\|\|_\infty$	$\|\|\nabla \cdot \mathbf{E}\|\|_\infty$
sib1	40	$1.1e-2$	$7.9e-3$	$5.6e-3$	$4.0e-3$
sib2	80	$8.1e-4$	$5.6e-4$	$4.0e-4$	$4.2e-4$
sib4	160	$5.4e-5$	$3.7e-5$	$2.7e-5$	$5.4e-5$
rate		3.84	3.87	3.86	3.10

Maximum errors at $t = 3$.

The finest grid has 6.5 million grid points.

Scattering of a plane wave by a dielectric cylinder

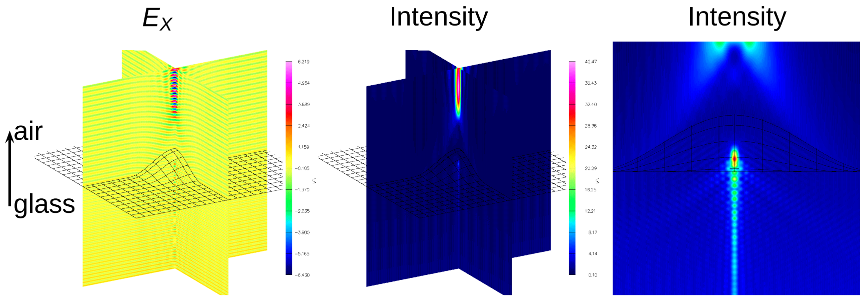




grid	$\|\|e^{E_x}\|\|_\infty$	$\|\|e^{E_y}\|\|_\infty$	$\|\|e^{H_z}\|\|_\infty$	$\delta_{\mathbf{E}}$
$\mathcal{G}_1$	$1.4e{-1}$	$2.9e{-1}$	$3.0e{-1}$	$6.7e{-2}$
$\mathcal{G}_2$	$1.0e{-2}$	$2.1e{-2}$	$2.2e{-2}$	$4.5e{-3}$
$\mathcal{G}_4$	$6.8e{-4}$	$1.4e{-3}$	$1.4e{-3}$	$2.9e{-4}$
rate σ	3.86	3.87	3.88	3.92

Known solution as a Mie series. Maximum errors at $t = 1$.

Scattering by a 3d material interface

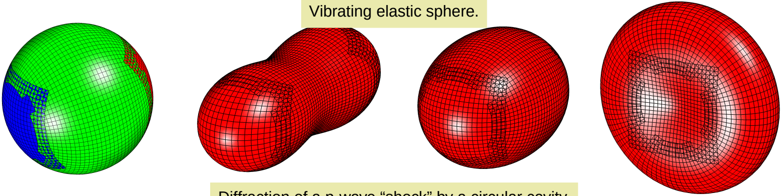


- Uses newly developed 4th-order accurate 3D material interface approximations.
- Scattering of a plane wave by an interface with a bump, glass-to-air.
- 1 billion grid points, 32 nodes (8 processors per node) of a Linux cluster.

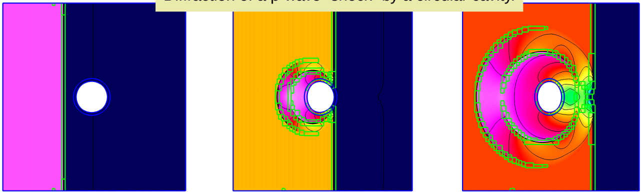
Cgsm: a solid-mechanics solver (in Overture.v24).

- linear elasticity on overlapping grids, with adaptive mesh refinement,
- conservative finite difference scheme for the second-order system,
- upwind Godunov scheme for the first-order-system.

Vibrating elastic sphere.



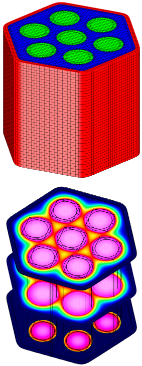
Diffraction of a p-wave “shock” by a circular cavity.



- D. Appelö, J.W. Banks , WDH, D.W. Schwendeman, *Numerical Methods for Solid Mechanics on Overlapping Grids: Linear Elasticity*, LLNL-JRNL-422223, submitted.

Cgmp: a multi-domain multi-physics solver.

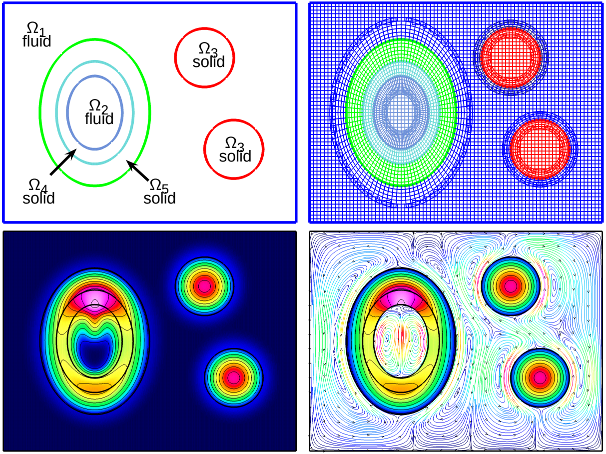
Conjugate heat transfer: coupling incompressible flow to heat conduction in solids.



- overlapping grids for each fluid or solid domain,
- a partitioned solution algorithm (separate physics solvers in each sub-domain),
- (cgins) incompressible Navier-Stokes equations (with Boussinesq approximation) for fluid domains,
- (cgad) heat equation for solid domains,
- a key issue is interface coupling.

• WDH., K. K. Chand, *A Composite Grid Solver for Conjugate Heat Transfer in Fluid-Structure Systems*, J. Comput. Phys, 2009.

The multi-domain composite grid approach for CHT



Each fluid or solid sub-domain is covered by an overlapping grid.
Fluid sub-domains : cgins. Solid sub-domains: cgad.
Coupled problem: cgmp.

Deforming composite grids for FSI

Goal: Couple overlapping grid techniques for modeling fluids and gases (using moving grids and AMR) with linear and non-linear solid mechanics codes.

Approach:

- Fluids: Overlapping grid fluid-mechanics solver.
- Solids : unstructured grid or overlapping-grid solid-mechanics solver.
- Boundary fitted deforming grids are used at the fluid-solid interfaces.

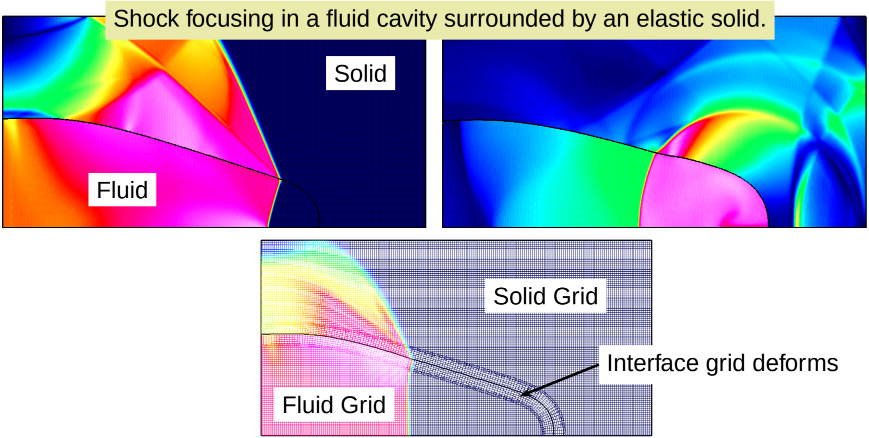
Strengths of the approach:

- Maintains high quality grids for large deformations and displacements.
- Uses efficient structured grid methods optimized for Cartesian grids.

Current status:

- Solve Euler equations in the fluid domains on moving grids.
- Solve equations of linear elasticity in the solid domains.
- Fluid grids at the interface deform over time.

Deforming composite grids for FSI



- Solving the Euler equations in the fluid, linear elasticity in the solid.

The figures show results from preliminary work to model an experiment by Veronica Eliasson.

Conclusions

- Overlapping grids have been used to solve a wide class of problems.
- Smooth boundary fitted grids for accuracy.
- Structured grids for efficiency.
- Rapid grid generation for moving geometry.
- Overture is a toolkit for grid generation and solving PDEs.
- The CG set of PDE solvers solve a variety equation in contiuum mechanics .

Open problem: automatic grid generation for complex geometry.